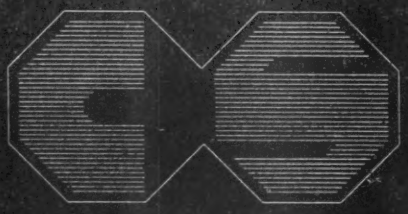

Journal of The Chemical Society

# Perkin Transactions II

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## 1978

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Abbreviations, symbols, and formulae are generally not permitted, and it is usual to spell out terms where necessary.

Reference to the preceding part of a series must be made as the reference (numbered 1) to the title in the form: ' The Chemistry of Vitamin $B_{12}$. Part VIII.[1] Controlled Potential Reduction of Vitamin $B_{12a}$.' [Reference to a preceding part in the references is in the form: Part VII, H. A. O. Hill, B. E. Mann, J. M. Pratt, and R. J. P. Williams, *J. Chem. Soc.* (*A*), 1968, 564. If the page number is unknown because the paper has still to be accepted, or is in the press, the paper number should be given.]

*Summary.*—Every paper for the *Journal* must be accompanied by a summary (50—250 words) setting out briefly and clearly the objects and results of the work. The summary should give a reader a clear idea of what the work has achieved and should be *independent* of the main text. This last point is of particular importance in connection with the names of compounds which, although they may be accompanied by a number which refers to a displayed formula in the body of the text, must be comprehensible without reference to this formula. Thus,

> Apetalactone, a new triterpene lactone isolated from *Calophyllum apetalum* Willd. has been shown to be 4,28-dihydroxy-3,4-secofriedelan-3-oic acid lactone (IIa).
>
> or
>
> Reaction of sodium hydride with ω-hydroxyalkyltriphenylphosphonium salts $Ph_3P^+[CH_2]_nOH\ X^-$ (I) has been investigated. The salt (I; $n = 1$, X = 1) gave triphenylphosphine and formaldehyde. The salt (I; $n = 2$, X = 1) gave triphenylphosphine oxide and ethylene. Similar reactions were carried out with ω-hydroxyalkyltriphenylarsonium (XIV) and ω-hydroxyalkyldimethylphenylammonium (XV) salts.

The summary should concern only the main subject of the work and its main conclusions; details of an involved argument or synthesis should not be included and, although classes of compounds prepared or discussed should be given rather than a list of compounds, key compounds in the work should be referred to.

*Introduction.*—This should give clearly and briefly, with relevant references, both the nature of the problem under investigation and its background.

*Results and Discussion.*—It is usual for the results to be presented first, and for them to be followed by a discussion of their significance. Only relevant results should be presented, and figures, tables, and equations should be used only for purposes of clarity and brevity. Data must not be reproduced in more than one form, *e.g.* in both figures and tables.

*Experimental Section.*—Descriptions of experiments should be given in detail sufficient to enable experienced experimental workers to repeat them; the degree of purity of materials should be given, as should the relative quantities used. Descriptions of established procedures are unnecessary. Standard techniques and methods used throughout the work should be stated at the beginning of the section. Apparatus should be described only if it is non-standard; commercially available instruments are referred to by their stock numbers (*e.g.* Perkin-Elmer 137 or Unicam SP 500 spectrophotometers). The accuracy of primary measurements should be stated. Unexpected hazards encountered during the experimental work should be noted. The detailed treatment of the Experimental section is dealt with in a forthcoming Notice to Authors.

*Acknowledgements.*—Contributors, other than co-authors, are acknowledged in a separate paragraph at the end of the paper; acknowledgements should be as brief as possible. Titles, Mr., Mrs., Miss, Dr., Professor, *etc.*, are given; degrees are not given. Organizations which operate on a commercial basis are not acknowledged.

*Bibliographic References.*—These are given on a separate sheet at the end of the manuscript and are referred to in the text by superior roman numerals. They must be distinguished from footnotes which are given at the bottom of the page to which they refer; they are referred to by an asterisk (*), dagger (†), *etc.* Bibliographic references and footnotes are the subject of Notice No. 3.

## General Detail

*Type Size.*—It should be noted that since the Experimental section and the results are printed in smaller type than the theoretical part, division between the two should be clear-cut and frequent alternation is not advisable.

*Brevity.*—Because of the large volume of work submitted for publication, brevity in the presentation of papers is essential and, for this reason, certain tendencies are discouraged; these are as follows:

(*a*) Unnecessary division of work into separate parts of a series. Papers are in no way discouraged solely on grounds of length.
(*b*) Submission of fragmentary work when this can be included in a larger communication.
(*c*) Historical introductory paragraphs in cases when a simple statement of the accepted present position suffices.
(*d*) Undue elaboration of hypotheses.
(*e*) Over-detailed and verbose exposition of ideas.
(*f*) Excessive use of diagrams, for example, straight-line plots that can be adequately expressed as an equation together with, if necessary, a table of deviations.
(*g*) Duplication of data as between text, tables, and figures, *etc.*

(*h*) Details of the preparation of simple derivatives such as esters, ethers, semicarbazones, *etc.*, and slight variations of essentially the same technique. (Unless the conditions are critical, quantities are superfluous, and only an indication of reagents and/or conditions is required.)

*Spelling.*—Standard English spelling is used (*Oxford English Dictionary*), although latitude with respect to alternative spellings for certain words is allowed. Where one form or the other of a particular spelling is adopted it should be used consistently throughout a paper.

*Punctuation.*—Although punctuation follows standard English practice, the following conventions are observed:

(*a*) A comma is placed before ' and ' or ' or ' in a series such as ' oxygen, sulphur, and selenium ' or ' $\lambda_{max.}$ 237, 295, and 343 nm.'

(*b*) Parentheses, square brackets, and braces are used, as necessary, in that order, *i.e.* {[( )]}.

(*c*) When a word is followed by a punctuation mark the parenthetical phrase must be inserted before the latter, *e.g.* ' m.p. 234° (decomp.),' and not ' m.p. 234°, (decomp.)'.

(*d*) A colon is used to separate a ratio, as in 1 : 20 —not a solidus 1/20.

(*e*) Parenthetical expressions of the same physical quantity in different units are separated by a comma (3·9 g, 0·1 mol) (30 ml, 1 mol); expressions of different physical quantities are separated by a semicolon (2·9N; 30 ml) (*d* 0·88; 8 ml).

*Hyphenation.*—Hyphens are used for two purposes: to divide and to compound.

*Division.* It is common practice to divide words, particularly when in a sequence, when one part is common to several of the words; in such cases, the hyphen, representing the point of attachment to the common part, is always inserted, *e.g.* ' the chloro-, bromo-, and fluoro-naphthacenes,' ' the *o-*, *m-*, or *p*-nitrotoluenes,' or ' the oxo-naphthalenes and -naphthacenes.' It is not good practice, however, to detach both a common prefix and a common suffix in a series, *e.g.* ' the dihydroxy- naphthalene- and phenanthrene-diones,' since confusion can arise.

' Sections ' of class names such as diazo-ketone, alkyl-diamine, epoxy-nitro-sulphone, *etc.*, are linked by hyphens.

It is also Society usage to insert a hyphen after a prefix which ends in a vowel or y; the hydroxy-group, the aza-function, the carboxy-compounds, the nitro-derivatives, but the methyl group (note that hydroxy, acetoxy, carboxy, ethoxy, and methoxy are used and not hydroxyl, acetoxyl, carboxyl, ethoxyl, and methoxyl).

It is customary to separate a pair of the same letter when these letters (in the same fount) would not naturally fall together, *e.g.* butyl-lithium, iodo-octane.

*Compounding.* A hyphen is often necessary when words are compounded to form a single modifying adjective to precede the noun being modified, thus: ' a melting-point determination ' or ' a free-radical chain mechanism.' A hyphen is not needed when adverbs are compounded, as in ' an electrically heated oven,' or for two-word chemical names such as ' nitric acid solution.'

*Miscellaneous uses of hyphens.* Hyphens are used to set apart numbers, configurational letters, Greek letters, and italicized prefixes: 1,2,5-trimethylcyclohexane, D-*gluco*-hexose, *s*-trinitrobenzene, β-chlorophenethylbenzene, tri-μ-carbonyl-bis(tricarbonyliron), and 3-methylpent-*trans*-2-ene.

*Use of Italics.*—As described below, italics are indicated in a typescript by single underlining. Particular attention should be paid to the following uses.

(*a*) Foreign words and phrases and Latin abbreviations are given in italics: *e.g.*, *in toto*, *in vivo*, *ca.*, *cf.*, *i.e.*, *etc.*

(*b*) In the names of chemical compounds or radicals italics are used for prefixes (other than numerals or symbols) when they define the position of named substituents, or when they define stereoisomers: other prefixes are printed in roman. (*Note:* Initial capital letters are not to be used with italic prefixes or single-letter prefixes: full points are not to be associated with letter prefixes.)

*o-*, *m-*, and *p*-nitrotoluenes, but *ortho-*, *meta-*, and *para*-compounds (*o-*, *m-*, and *p-* are used only with specific names; *ortho-*, *meta-*, and *para-* are used with classes), *s*-trinitrobenzene, *NN*-dimethylaniline, *trans-* and *cis*-hexane-1,2-diol, *gem-* and *vic*-diols, benzil *anti*-oxime, 3-*O*-methyl-L-*glycero*-tetrulose.

At the beginning of a sentence the first roman letter after the prefix is capitalized: ' D-*glycero*-D-*gluco*-Heptose was subjected . . . ' and ' β-*p*-Tolylchalcone gave . . . '

(*c*) The scientific names of genera, species, and varieties are italicized.

(*d*) In references to periodicals their names or abbreviations are set in italics.

*Note:* Greek letters are not italicized, and should not therefore be underlined in typescripts.

*Headings.*—(*a*) Main sections (Experimental, Discussion, *etc.*): side-heading, small capitals, no final fullstop.

(*b*) Main side-heading: italics, initial capital letter for each noun and adjective, final fullstop and dash.

(*c*) Subsidiary side-heading: italics, first initial capital only, final fullstop but no dash.

(*d*) Further subdivision: by italic (*a*), (*b*), *etc.* (no following fullstop), and finally (i), (ii), *etc.* If (a), (b), *etc.* are used in front of a subsidiary side-heading, then for contrast these letters are not italicized.

Letters and prefixes which are ordinarily printed in italics are transferred for contrast into roman type in italicized phrases (see example below, where *O*-alkyl becomes O-*alkyl*).

Physicochemical symbols, however, remain in their prescribed form, and numerals and Greek letters are not italicized.

*Examples:*

EXPERIMENTAL

*Preparation of Aliphatic Aldoximes and Ketoximes.—Acetoxime* O-*alkyl ethers.* (*a*) Acetoxime (100 g) was dissolved . . .

*Density* (*d*) *of the Alcohol at* 295 K.—The series of aliphatic alcohols . . .

*Note:* In the above examples it should be noted that the type of print required to indicate italics, capitals, small capitals, *etc.* is shown by underlining; this convention must be strictly adhered to, *i.e.*

Single underlining for *italic* type

Double underlining for SMALL CAPITALS

Treble underlining for ORDINARY CAPITALS

Wavy underlining for **bold black** type

# NOTICES TO AUTHORS—No. 3/1968

## Bibliographic References and Footnotes

A clear distinction is made between bibliographic references and footnotes. The latter are used to present material which, if included in the body of the text, would disrupt the flow of the argument but which is, nevertheless, of importance in qualifying or amplifying the textual material. Such footnotes are referred to with the following symbols: *, †, ‡, §, ¶, ‖, *etc.* [*Note:* Since an asterisk is used to indicate the author to whom correspondence should be addressed, its use early on in a paper is not advised; a dagger (†) is preferred.]

*Bibliographic References.*—Reference to the source of statements in the text is made by use of *superior numerals* at the appropriate place. The references themselves are given as footnotes at the bottom of the corresponding page in the final printed text. It is thus *essential* that bibliographic references are numbered in the order in which they will appear.

When citation of a paper is repeated the numeral previously given to that reference is to be used also at the second citation; the footnote is not repeated.

The position of the superior numeral should be chosen with care, particularly when it does not follow an author's name. If placed adjacent to punctuation, the numeral should normally be placed after the punctuation mark, *e.g.* 'This compound was shown to be the dienone,[3] which . . . '. It may be necessary to modify this rule, however, to avoid confusion, thus: 'In this way the method was found to be suitable for lead[2], tin[3], bismuth[4], and mercury[5].'

Particular care is necessary where a reference number is likely to be confused with a superscript numeral indicating a power index: '. . . which gave a value of 2·3 $cm^3$ . . . ' should be written as '. . . which gave a value[3] of 2·3 cm' or '. . . which gave a value of 2·3 cm (ref. 3)'.

Since it is usually difficult to print a table in a given position in the text, references within the table are best dealt with by taking the individual references into the printed footnotes to the tables and using a new reference number sequence therein. Should the references cited in the tables appear much earlier in the text, these earlier reference numbers may be used.

*Journals.* New instructions for the abbreviation of journal titles will be issued early in 1980. At the present time where authors have difficulty in deciding on a suitable journal abbreviation they are invited either to write directly to the Editors or to consult current copies of the *Journal.*

*Books.* Titles of books are cited in quotation marks, in upright letters, and the author(s), title, publisher, town, date (or edition, if more than one has been published), and page number (if required) must be given in that order:

C. J. M. Stirling, 'Radicals in Organic Chemistry,' Oldbourne Press, London, 1965, p. 69.

T. J. Suen, in 'Polymer Processes,' ed. C. E. Schildknecht, Interscience, New York, 1956, vol. X, p. 295.

*Patents.* Patents should be indicated in the form: B.P. 367,450, 367,455-7. U.S.P. 1,171,230. G.P. 436,112-4. Jap.P. 20,101. Dates are indicated thus: B.P. 666,776/1956. Patents which are applied for must always be given a year, *e.g.* B.P. Appl. 102/1968.

*Reports and Bulletins,* etc.

R. A. Allen, D. B. Smith, and J. E. Hiscott, 'Radioisotope Data,' UKAEA Research Group Report AERE-R 2938, H.M.S.O., London, 1961.

'Collected Papers on Methods of Analysis for Uranium and Thorium,' Geological Survey Bulletin 1006, U.S. Government Printing Office, Washington D.C., 1954.

*Material presented at meetings.*

N. N. Greenwood, Abstracts, Anniversary Meeting of the Chemical Society, Glasgow, 1965, C1.

N. S. Anderson and D. A. Rees, in 'Proceedings of the Vth International Seaweed Symposium,' ed. E. G. Young and J. L. McLachlan, Pergamon Press, Oxford, 1966, p. 405.

*Theses.*

A. D. Mount, Ph.D. Thesis, University of London, 1967.

*Reference to unpublished material.* For material presented at a meeting, congress, or before a society, *etc.*, but not published, the following form is used:

[1] A. R. Jones, presented in part at the XXth Congress of the International Union of Chemistry, Paris, September, 1960.

For material accepted for publication, but not yet published, the following form is used:

[2] A. R. Jones, *J. Amer. Chem. Soc.*, in the press.

If the paper has been submitted to the Society, the paper number should be given:

[3] A. R. Jones, *J. Chem. Soc.* (*A*), in the press (8/556).

For material submitted for publication but not yet accepted the following form is used:

[4] A. R. Jones, submitted for publication in *Angew. Chem.*

For personal communications the following form is used:

[5] G. B. Ball, personal communication. (*Note:* the form, G. B. Ball, private communication, is inappropriate.)

If material is to be published but has yet to be submitted the following form is used:

[6] Unpublished data.

*Names.*—The names and initials of all authors are always given in the reference footnote; they must not be replaced by the phrase *et al.* This does not prevent some, or all, of the names being mentioned at their first citation in the cursive text: initials are not necessary in the text.

For Chinese and Spanish authors all names should be given as in the original, since the patronymic is not always given last in these languages. If co-authors are to be collectively cited, as in 'Smith and his co-workers' or 'Smith *et al.*,' the latter form is inappropriate unless the individual name 'Smith' appears first among the authors named in the original.

*Composite References.*—Whenever possible, composite references should be used rather than a series of individual references. The style for composite references is as follows:

[1] A. B. Jones, *J. Chem. Soc.* (*A*), 1967, 234.

[2] A. B. Jones, *J. Chem. Soc.* (*A*), 1966, 123; 1967, 234.

[3] A. B. Jones, *J. Chem. Soc.* (*A*), 1966, 123; *J. Amer. Chem. Soc.*, 1956, **78**, 1234.

[4] A. B. Jones, *J. Chem. Soc.*, 1956, 234; A. B. Jones and C. D. Brown, *J. Chem. Soc.* (*B*), 1967, 234, 1077; 1968, 599.

[5] A. B. Jones, *J. Amer. Chem. Soc.*, 1956, **78**, 1234; A. B. Jones and C. D. Brown, *ibid.*, 1957, **79**, 567; A. B. Jones and E. F. Green, *ibid.*, p. 999.

If only one paper from a composite reference is required for citation later, then two numbers may be assigned to the first citation (*e.g.* Jones [1,2]); alternatively, long composite references may be divided by letters, *e.g.*:

(*a*) A. B. Jones, *J. Chem. Soc.* (*A*), 1954, 467; (*b*) A. B. Jones and C. D. Brown, *J. Chem. Soc.* (*B*), 1967, 234.

A. B. Jones, *J. Chem. Soc.* (*A*), (*a*) 1953, 267; (*b*) 1954, 1742; (*c*) *etc.*

A composite reference may cite a previous reference in the form:

[12] A. B. Jones, *J. Chem. Soc.*, 1956, 234; C. D. Brown, ref. 5.

(*Note: ibid.* is used only within a given reference and not to refer from one reference number to another: the abbreviated title for the journal should be repeated for separate reference numbers.)

*Idem, loc. cit.*, and *op. cit.* are not used in references.

# NOTICES TO AUTHORS—No. 5/1969

## The International System of Units (SI)

### Preamble

For many years the practice of The Society in respect of units has been based on the recommendations of a joint Committee of The Royal Society, The Chemical Society, The Faraday Society, and The Physical Society. The 1951 set of recommendations published by that Committee formed the basis of Chapter 7 of the 'Handbook for Chemical Society Authors' but since their promulgation much effort has been expended in international circles to devise and approve a basic set of coherent units. This having been completed, The Joint Symbols Committee of The Royal Society, of which The Chemical Society is a participating member, has produced a completely new set of recommendations in a pamphlet 'Symbols, Signs and Abbreviations' 1969 (copies of this pamphlet or further details can be obtained from the Managing Editor, The Chemical Society, Burlington House, London, W1V OBN). The basis of the new recommendations is the 'Système International d'Unités' (to be abbreviated to SI, in all languages).

The advantages offered by SI are as follows.

(i) It is a truly coherent system, *i.e.* the product or quotient of any two unit quantities in the system is the unit of the resultant quantity. This contrasts with the previous situation where, even in metric systems used within the same discipline, many additional units are arbitrarily and sometimes differently defined.

(ii) SI derives nearly all the quantities needed in all sciences and technologies from a very small set of base-units.

(iii) The variety of multiples and sub-multiples in common use is minimized.

(iv) A more uniform presentation can be ensured.

(v) Presentation is such that the relation of any derived unit, or multiple or sub-multiple of a derived unit, to the coherent unit is always obvious and simple.

### Policy

(1) The Society announces its approval and support of SI, and its intention that SI shall become the preferred system in its publications.

(2) *Guidelines for the publications of the Society.* The Society realises that public acceptance of this system will be more a matter of education and tolerance than of dictatorial action. It nevertheless desires that the SI system and units compatible with it shall *rapidly* become the established standard in the Society's publications. An author will not be denied any reasonable usage, but if non-SI units are used for critical data or for quantities measured to a high order of accuracy (as opposed to the rough physical conditions of an experiment), the definitive values will be expressed in SI units as well.

The following will be the guidelines used:

(*a*) A metric system will always be used in preference to a non-metric one.

(*b*) The SI system will be the standard usage.

(*c*) The units used to record the *definitive* values of 'critical data' or quantities measured to high degree of accuracy will be of the SI system.

(*d*) When non-SI units are used they must be adequately explained unless their definition is obvious (*e.g.* degree Celsius, mmHg, g, h). The derivation of derived non-SI units will be indicated.

(*e*) Equations involving electrical quantities should normally be those appropriate for use with SI (rationalized m.k.s) units. If authors wish to use equations suitable for e.s.u. or e.m.u. the lack of consistency with SI units must be explicitly noted.

(3) *The principal changes.* There are four of these:

(*a*) Basic units: the metre and the kilogramme replace the centimetre and the gramme of the old metric system.

(*b*) The unit of force is now the newton (kg m $s^{-2}$).

(*c*) The unit of energy is the joule and of power the joule per second (watt); thus the variously defined calories and non-metric units of energy and power are superseded.

(*d*) 'Electrostatic' and electromagnetic' units are replaced by SI electrical units.

### Detail

(4) *Definition.* A quantity is expressed as the product of a numerical value and a unit.

(5) *The System.* The fully coherent SI consists of base-units, supplementary units, derived units, and decimal multiples and sub-multiples of these units, formed by use of prefixes only.

(6) *Coherent systems.* A coherent system is one based on a selected set of 'base-units' from which 'derived units' are obtained by multiplication without introducing numerical factors.

(7) *Base-units.* The name International System of Units (SI) was adopted by the Conférence Générale de Poids et Mesures in 1960 for the coherent system now based on the base-units given in Table 1.

TABLE 1

| *Physical quantity* | *Name of base-unit* | *Symbol for unit* |
|---|---|---|
| length | metre | m |
| mass | kilogramme | kg |
| time | second | s |
| electrical current | ampere | A |
| thermodynamic temperature | kelvin | K |
| luminous intensity | candela | cd |
| amount of substance | mole | mol |

(8) *Supplementary units.* The SI also includes two 'supplementary' *dimensionless* units as follows:

| *Physical quantity* | *Name of unit* | *Symbol for unit* |
|---|---|---|
| plane angle | radian | rad |
| solid angle | steradian | sr |

(9) *Multiples and sub-multiples.* In the SI there is one and only one basic unit for each physical quantity. Decimal fractions and multiples of these basic units may, however, be constructed by use of certain prefixes (see Table 2). They may also be used with derived SI units.

TABLE 2

| *Fraction* | *Prefix* | *Symbol* | *Multiple* | *Prefix* | *Symbol* |
|---|---|---|---|---|---|
| $10^{-1}$ | deci | d | 10 | deka | da |
| $10^{-2}$ | centi | c | $10^{2}$ | hecto | h |
| $10^{-3}$ | milli | m | $10^{3}$ | kilo | k |
| $10^{-6}$ | micro | $\mu$ | $10^{6}$ | mega | M |
| $10^{-9}$ | nano | n | $10^{9}$ | giga | G |
| $10^{-12}$ | pico | p | $10^{12}$ | tera | T |
| $10^{-15}$ | femto | f | | | |
| $10^{-18}$ | atto | a | | | |

The combination of a prefix and a unit symbol constitutes a new single unit symbol; compounding of prefixes is not permitted.

Although it will not always be possible, particularly in Tables, the general principle should be to choose a unit (*i.e.* including multiple or sub-multiple) such that the resulting numerical value is between 0·1 and 1000.

(10) *Derived units.* Some derived units have special names and symbols, and these are given in Table 3.

TABLE 3

| *Physical quantity* | *Name of SI unit* | *Symbol for SI unit* | *Definition of SI unit* |
|---|---|---|---|
| energy | joule | J | $kg\ m^2\ s^{-2}$ |
| force | newton | N | $kg\ m\ s^{-2} = J\ m^{-1}$ |
| power | watt | W | $kg\ m^2\ s^{-3} = J\ s^{-1}$ |
| electric charge | coulomb | C | A s |
| electric potential difference | volt | V | $kg\ m^2\ s^{-3}A^{-1} = JA^{-1}\ s^{-1}$ |
| electric resistance | ohm | Ω | $kg\ m^2\ s^{-3}A^{-2} = VA^{-1}$ |
| electric capacitance | farad | F | $A^2\ s^4\ kg^{-1}\ m^{-2} = As\ V^{-1}$ |
| magnetic flux | weber | Wb | $kg\ m^2\ s^{-2}A^{-1} = V\ s$ |
| inductance | henry | H | $kg\ m^2\ s^{-2}A^{-2} = VA^{-1}\ s$ |
| magnetic flux density | tesla | T | $kg\ s^{-2}A^{-1} = V\ s\ m^{-2}$ |
| luminous flux | lumen | lm | cd sr |
| illumination | lux | lx | $cd\ sr\ m^{-2}$ |
| frequency | hertz | Hz | $s^{-1}$ |

*Others do not*

| *Physical quantity* | *SI unit* | *Symbol for SI unit* |
|---|---|---|
| area | square metre | $m^2$ |
| volume | cubic metre | $m^3$ |
| density | kilogramme per cubic metre | $kg\ m^{-3}$ |
| velocity | metre per second | $m\ s^{-1}$ |
| angular velocity | radian per second | $rad\ s^{-1}$ |
| acceleration | metre per second squared | $m\ s^{-2}$ |
| pressure | newton per square metre | $N\ m^{-2}$ |
| kinematic viscosity, diffusion coefficient | square metre per second | $m^2\ s^{-1}$ |
| dynamic viscosity | newton second per square metre | $N\ s\ m^{-2}$ |
| electric field strength | volt per metre | $Vm^{-1}$ |
| magnetic field strength | ampere per metre | $A\ m^{-1}$ |
| luminance | candela per square metre | $cd\ m^{-2}$ |

(11) *Symbol.* The symbol for a unit will be printed in roman (upright) type, remains unaltered in the plural and does *not* take a full point, *i.e.* 5 cm not 5 cm. or 5 cms or 5 cms.

The symbol will be separated from the numerical value by a thin space.

(12) *Decimal fractions and multiples of SI units having special names.* These names are not part of the SI, but for the time being their use in The Society's publications may continue. The list given in Table 4 is not exhaustive.

TABLE 4

| *Physical quantity* | *Name of unit* | *Symbol unit* | *Definition of unit* |
|---|---|---|---|
| length | ångström | Å | $10^{-10}\ m = 10^{-1}\ nm$ |
| length | micron | $\mu m$ | $10^{-6}\ m$ |
| area | barn | b | $10^{-28}\ m^2$ |
| volume | litre | l | $10^{-3}\ m^3 = dm^3$ |
| mass | tonne | t | $10^{3}\ kg = Mg$ |
| force | dyne | dyn | $10^{-5}\ N$ |
| pressure | bar | bar | $10^{5}\ N\ m^{-2}$ |
| pressure | pascal | Pa | $Nm^{-2}$ |
| energy | erg | erg | $10^{-7}\ J$ |
| kinematic viscosity diffusion coefficient | stokes | St | $10^{-4}\ m^2\ s^{-1}$ |
| dynamic viscosity | poise | P | $10^{-1}\ kg\ m^{-1}\ s^{-1}$ |
| magnetic flux | maxwell | Mx | $10^{-8}\ Wb$ |
| magnetic flux density (magnetic induction) | gauss | G | $10^{-4}\ T$ |
| conductance | siemens | S | $\Omega^{-1}$ |

(13) *Units defined in terms of the best available experimental values of certain physical constants.* These units are not part of the SI. The factors for conversion of these units to SI units are subject to change in the light of new experimental measurements of the constants involved. Their use outside the restricted contexts to which they are appropriate should be discouraged. The following list is not exhaustive.

| *Physical quantity* | *Name of unit* | *Symbol for unit* | *Conversion factor* |
|---|---|---|---|
| energy | electronvolt | eV | $eV \approx 1{\cdot}6021 \times 10^{-19}\ J$ |
| mass | unified atomic mass unit | u | $u \approx 1{\cdot}660\,41 \times 10^{-27}\ kg$ |

(14) *Other units now exactly defined in terms of the SI units.* These units are not part of the SI. It is recognized that their use may be continued for some time but it is recommended that except in special circumstances they should be progressively abandoned in conformity with international recommendations. The list given in Table 5 is by no means exhaustive. Each of the definitions given in the fourth column is *exact.*

TABLE 5

| *Physical quantity* | *Name of unit* | *Symbol for unit* | *Definition of unit* |
|---|---|---|---|
| length | inch | in | $2{\cdot}54 \times 10^{-2}\ m$ |
| mass | pound (avoirdupois) | lb | 0·453 592 37 kg |
| time * | minute | min | 60 s |
| time * | hour | h | 3600 s |
| force | kilogramme-force | kgf | 9·806 65 N |
| force | pound-force | lbf | $9{\cdot}806\ 65 \times 0{\cdot}453\ 592\ 37\ N$ |
| pressure | atmosphere | atm | $101\ 325\ N\ m^2$ |
| pressure | conventional millimetre of mercury | mmHg | $13{\cdot}5951 \times 9{\cdot}806\ 65\ N\ m^{-2}$ |
| pressure | torr | Torr | $(101\ 325/760)\ N\ m^{-2}$ |
| pressure | pound-force per square inch | $lbf\ in^{-2}$ | $\frac{9{\cdot}806\ 65 \times 4535{\cdot}9237}{6{\cdot}4516}\ N\ m^{-2}$ |
| energy | kilowatt hour | kW h | $3{\cdot}6 \times 10^{6}\ J$ |
| energy | thermochemical calorie | cal(thermochem.) | 4·184 J |
| energy | I.T. calorie | $cal_{IT}$ | 4·1868 J |
| thermodynamic temperature | degree Rankine | °R | (5/9) K |
| radioactivity | curie | Ci | $3{\cdot}7 \times 10^{10}\ s^{-1}$ |

* Use of other common units (min, h, day) may continue in normal expressions of intervals of time.

# NOTICE TO AUTHORS—No. 6/1969

## Formulae and Figures

The purpose of all illustrative matter in a paper is to clarify the arguments and descriptions rather than to duplicate them. The Society strongly encourages the use of displayed formulae, particularly in the form of schemes where the details of a reaction sequence are often more easily understood when illustrated than when described in the text.

All formulae and figures should be clearly drawn, and in the case of figures provided with captions; the latter should be typed on a separate sheet. Since all formulae carry a key number by which they are identified, unless they form part of the running text or unless they are part of a scheme which itself has a caption, they are not generally further described. Blocks of formulae do not need a caption.

Illustrative matter is divided, for technical reasons, into figures and formulae, although in many cases (*e.g.* crystal structures which may be regarded as formulae but which are treated as figures) these divisions overlap.

*Structural Formulae.*—(*a*) Only those formulae which are displayed may be given key numbers. In all other cases the compounds concerned are referred to by name only.

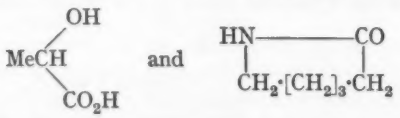
(*b*) Formulae are numbered sequentially with bold arabic numerals in parentheses [(**1**), (**2**), and (**3**) *etc.*] as they are displayed and *not* as they are mentioned in the text.

(*c*) In complex reaction schemes the formulae should be numbered serially following the reaction sequence. Non-sequential numbering in a collection of formulae can render it hard to locate an individual number.

(*d*) Structural or displayed formulae must be carefully and accurately drawn or typed on a separate sheet, rather than inserted into the text, although a marginal indication of where they are to go in the text is desirable.

(*e*) Formulae inserted into the body of the text (as distinct from those displayed separately) should be written on one line if possible, *e.g.*

$HO{\cdot}CHMe{\cdot}CO_2H$ and $\overline{NH{\cdot}[CH_2]_5{\cdot}CO}$ rather than



(*f*) Points (which may be typed as full stops) are used to indicate bonds between the atoms of the backbone chain of a compound. The symbol of each element of that chain is preceded by a full stop (or colon for a double bond) and followed by the symbols or formulae of the atoms or groups that are attached to it (parentheses being used where necessary to enclose compound groups), *e.g.* *o*-$HO{\cdot}C_6H_4{\cdot}CH_2{\cdot}NH_2$ and $CH_2Cl{\cdot}CH(OH){\cdot}CO_2H$.

Groups that are indicated by a single symbol (*e.g.* Me and Et *etc.*) do not need use of such full stops.

Repeating sequences of a backbone composite group are enclosed with square brackets and their number is indicated by an inferior multiplier, *e.g.* $HO{\cdot}[CH_2]_4{\cdot}NH_2$, but $HO{\cdot}[CH_2]_4{\cdot}N(CH_2{\cdot}OH)_2$.

(*g*) The use of large circles to represent six delocalized π-electrons in cyclic systems (with or without positive or negative signs as appropriate) is permitted in certain circumstances. Cyclic systems with more or less than six delocalized π-electrons may be represented by formulae containing dotted lines. Both topics are dealt with in *Proceedings*, 1959, 75.

(*h*) Customary steric conventions must be observed, notably for steroids, triterpenes, and carbohydrates. The Society uses wedges (◢) or heavy lines (—) rather than blocked circles (●) and broken lines in the form – – – – – rather than ıllı.

(*i*) The symbols Me, Et, $Pr^n$, $Pr^i$, $Bu^n$, $Bu^i$, $Bu^s$, $Bu^t$, Ph, Ac, Bz (the symbol for PhCO and not for $PhCH_2$), Alk, Ar, and Hal, should be used but may be written in full when the groups are involved in the reaction described. Other special symbols, if used, require an explanatory footnote. The carboxy-group is written $CO_2H$ (*not* COOH) and similarly $CO_2R$.

(*j*) One variable univalent substituent is indicated by R; when more than one independently variable general substituent is present, $R^1$, $R^2$, and $R^3$ should be used (*not* R, $R^1$, $R^2$, $R^3$; or $R_1$, $R_2$, and $R_3$ which indicate 1 × R and multiples of R thereof).

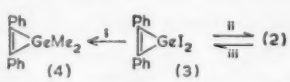
(*k*) Often it is desirable to use one formula to represent a number of related compounds (or classes of compounds) by the use of one or more independently variable substituents. It is preferable to give each compound thus represented a separate key number rather than to subdivide individual key numbers by alphabetical suffixes [*i.e.* (**1a**), (**1b**), (**1c**) *etc.*].

(**1**) $R^1 = R^2 = Ph$, $R^3 = Me$, X = O
(**2**) $R^1 = Me$, $R^2 = R^3 = Ph$, X = S

(**3**) $R^1 = Me$, $R^2 = Ph$, $R^3 = Bz$
(**4**) $R^1R^2 = CO{\cdot}O{\cdot}CO$, $R^3 = Ph$

The use of more than four independently variable substituents or atoms on one generalized formula is discouraged.

(*l*) Once a formula has been displayed it is permissible to employ its key number in later reaction schemes or equations rather than to re-display the formula:



Reagents: i, MeMgI; ii, NaOH; iii, HI

It should be noted that reagents and reaction conditions are given as footnotes to the scheme for economy of space; if present, an equation number is set as far to the right as possible, and if there is likelihood of

confusion with compound key-numbers it is accompanied by the word equation.

(*m*) Displayed formulae, unless they are capable of being typed on one line [see point (*e*) above], should not be included in tables; they should be displayed before the table with a key number for each compound and this should be used in the table.

(*n*) The key number for a compound may be used in the cursive text to avoid repetition of long chemical names; this device must not be used to excess. In general it is preferred if the key number is qualified by a partial name for the compound as in the following example:

' Pyolin (**1**) was oxidized by permanganate to the oxo-acid (**2**), the methyl ester (**3**) of which with methylmagnesium iodide gave the normal product (**4**) '.

(*o*) Reference to compounds in the Summary by key number alone is not allowed since a summary should be comprehensible without reference to the body of the paper itself. The reference number should, however, accompany the name of the compound to which it refers.

*Figures.*—(*a*) Figures must bear on the back the names of the authors, the title of the paper (abbreviated if necessary), and the number of the figure.

(*b*) Figures must be in Indian ink, on Bristol board, white smooth cartridge paper, tracing linen, plastic film (it is essential that the special plastic ink developed for this is used), or graph paper with *faint* blue lines (red or brown lines must not be present as these may be reproduced by the photographic process of block making). Since lines must be black and sharp, photostats or similar prints are often not suitable. If paper is used, it must be strong enough to withstand repeated handling.

(*c*) Lettering and numerals must be in *blue pencil* (*not* red or black pencil or ink) clearly legible but not so heavily scored as to make a permanent impression on the paper or board.

(*d*) When the figures are large (more than 8 in × 10 in), smaller copies (which may be rough, as long as they are clear) should be supplied for submission to the referees; editing will not be undertaken, however, before the final figures are received.

(*e*) Figures must be carefully drawn, preferably three times the size (linear) that seems necessary to ensure sharp printing, but excessive reduction is costly and illustrations that exceed five times the size of the finished block may be returned to the author for redrawing.

(*f*) Two-inch margins are essential all round figures. Lettering for insertion at margins should be placed well clear of the ordinate or abscissa line so that it can be copied before erasure.

Lettering and touching-up are done by the Society and clarity of instructions is essential. When there is much lettering, or complicated lettering, and always when tracing linen or plastic film is used, a rough tracing should be added with the lettering shown in ink.

(*g*) Since, for printing, the size is reduced, lines should not be too thin. Given lines must be of even thickness, angles neat, and curves smooth.

(*h*) Graphs should have only the requisite minimum of the scale (not less than three points) marked by numerals, and the scale lines should not normally be continued into the body of the figure.

(*i*) Graphs in any one paper should, when convenient, be drawn to the same scale, and scale markings should, when possible, be identical so that the graphs may be placed adjacent on the page. Contrariwise, two curves drawn to different scales can be shown on one graph by having the appropriate scales on the left-hand and the right-hand side. The use of both right- and left-hand axes and top and bottom axes on figures which have quantitative significance is encouraged.

(*j*) Experimental points must be shown sufficiently large to be distinguishable when reduced in size. Whenever possible, they should be confined to open and closed circles, crosses, squares, and triangles. Partly black circles and similar signs frequently become indistinguishable in print.

(*k*) Curves may be distinguished as full lines (——), broken (– – – –) or dotted lines (· · · ·), and dot-dash lines (— · — · —); further differentiation should normally be achieved by labelling the curves, which is, in any case, desirable.

(*l*) For reference in legends, it is preferable to mark curves A, B, C, *etc.* rather than to reproduce the type of line in print.

(*m*) There must be no unnecessary waste space, *e.g.* around curves; ordinates and abscissae should start at zero only if the curve extends to that range. Enlargement of parts of a figure can occasionally be placed in a corner of the complete figure.

(*n*) It is not advisable to insert much or complicated lettering on curves or in blank spaces; mistakes (in copying by the artist) can rarely be rectified once the block is made. It is better to label the curves A, B, C, *etc.* and to use explanatory legends.

(*o*) *Large* solid objects should be represented by hatching rather than by black surfaces, otherwise the ink may smear on printing.

(*p*) Photographs are reproduced by a half-tone process on art paper. The prints supplied must be very clear and of good contrast, as considerable definition may be lost in reproduction.

(*q*) Captions and explanatory legends, to be set by the printer should be typed on a separate page attached to the manuscript, and not given on the figure itself.

(*r*) Figures are numbered consecutively Figure 1, Figure 2, *etc.* (in arabic numerals). Photographs (half-tone reproduction) are numbered consecutively Plate 1, Plate 2, *etc.* but these numbers are independent of the numbering of any figures.

(*s*) Since figures represent an uneconomical use of space their number and size should be kept to a minimum. Figures and tables for the same values are discouraged.

# NOTICES TO AUTHORS—No. 7/1970 (revised 1976)

## Deposition of Data—Supplementary Publications Scheme

### Preamble

The growing volume of research that produces large quantities of data, the increasing facilities for analysing such data mechanically, and the rising cost of printing are all making it very difficult to publish in the *Journal* in the normal way the full details of the experimental data which become available. Moreover, whilst there is a large audience for the general method and conclusions of a research project, the number of scientists interested in the details, and in particular in the data, of any particular case may be quite small. The British Library, Lending Division (B.L.L.D.) in consultation with the Editors of scientific journals, has now developed a scheme whereby such data and detail may be stored and then copies made available on request at the B.L.L.D., Boston Spa. The Chemical Society is a sponsor of this scheme and has indicated to the B.L.L.D. its wish to use the facilities being made available in this ' Supplementary Publications Scheme '.

Bulk information (such as crystallographic structure factor tables, computer programmes and output, evidence for amino-acid sequences, spectra, *etc.*), which accompanies papers published in future issues of the Chemical Society's *Journal* may in future be deposited, free of charge, with the Supplementary Publications Scheme, either at the request of the author and with the approval of the referees or on the recommendation of referees and with the approval of the author.

### The Scheme

Under this scheme, authors will submit articles and the supplementary material to the *Journal* simultaneously in the normal way, and both will be refereed. If the paper is accepted for publication the supplementary material will be sent by the Society to the B.L.L.D. where it will be stored. Copies will be obtainable by individuals both in the U.K. and abroad on quoting a supplementary publication number that will appear in the parent article.

### Preparation of Material

Authors will be responsible for the preparation of camera-ready copy according to the following specifications (although the Society will be prepared to help in case of difficulty).

(*a*) Optimum page size for text or tables in typescript: up to 30 cm × 21 cm.
(*b*) Limiting page size for text or tables in typescript: 33 cm × 24 cm.
(*c*) Limiting size for diagrams, graphs, spectra, *etc.*: 39 cm × 28.5 cm.
(*d*) Tabular matter should be headed descriptively on the first page, with column headings recurring on each page.
(*e*) Pages should be clearly numbered.

It is recommended that all material which is to be deposited should be accompanied by some prefatory text. Normally this will be the summary from the parent paper and authors will greatly aid the deposition of the material if a duplicate copy of the summary is provided. If authors have the facilities available the use of a type face designed to be read by computers is encouraged.

### Deposition

The Society will be responsible for the deposition of the material with the B.L.L.D. The B.L.L.D. will not receive material direct from authors since the Library wishes to ensure that the material has been properly and adequately refereed.

### Action by the Society

The Society will receive a manuscript for publication together with any supplementary material for deposition and will circulate all of this to referees in the normal way. When the edited manuscript is sent to the printers the supplementary material will be sent for deposition to the B.L.L.D. The Society will add to the paper a footnote indicating what material has been deposited in the Supplementary Publications Scheme, the supplementary publication number, and details as to how copies may be obtained.

### Availability

Copies of Supplementary Publications may be obtained from the B.L.L.D. on demand by organizations which are registered borrowers. They should use the normal forms and coupons for such requests addressing them as follows:

Mr. J. P. Chillag,
British Library Lending Division,
Boston Spa,
Wetherby,
West Yorkshire, LS23 7BQ, U.K.

Non-registered users may also obtain copies of Supplementary Publications but should first apply for price quotations. These are available from the Loans Office at the above address.

## International Collaboration

A similar scheme (known as the National Auxiliary Publications Service) is being operated in the U.S.A. by the American Society for Information Science. Similar schemes are also being contemplated in other countries. The provision of reciprocal arrangements for the exchange of supplementary data between the various national deposition centres is being investigated.

## NOTICES TO AUTHORS—No. 8/1970

### *X*-Ray Crystallographic Structure Factor Tables

The Society has recently taken advice from the members of its Chemical Crystallography Group and as a result of this and of the inception of the National Lending Library Supplementary Publications Scheme (discussed in Notices to Authors No. 7) the following rules are being taken into use forthwith to govern the publication or deposition of *X*-ray crystallographic structure factor tables.

(i) The Society will no longer publish tables of structure factors in its publications except in accordance with the provision of paragraph (iv) below.

(ii) All authors of crystallography papers will submit along with the manuscript a readable table of such structure factors for the referees' inspection. The table should be prepared in accordance with the detail given in paragraph 3 of Notices to Authors No. 7 so that it may be used for deposition. Computer printout may be used providing that it is top copy in good contrast (see note).

(iii) If the referees accept the paper and its associated structure factor tables then the Society will deposit these structure factor tables in the National Lending Library Supplementary Publications Scheme (see Notices to Authors No. 7) and will publish as a footnote to the paper the necessary details that will enable any reader to obtain a copy in microfiche or an electrophotographic printoff of the data tables associated with the paper.

(iv) Authors, or the referees, may request publication of such tables of structure factors, *in extenso*, in cases that seem to them to be desirable. It is expected that this will occur only rarely.

(v) The details of the National Lending Library Supplementary Publications Scheme and the methods for obtaining photographic printoff of material deposited with that scheme are given in Notices to Authors No. 7.

*Note to paragraph* (*ii*). Structure factors tables prepared from computer printout must be presented in the form indicated in paragraph 3 of Notices to Authors No. 7 and must be arranged with the greatest economy of space possible [*i.e.* not less than two groups of columns ($h$, $k$, $l$, $F_c$, $F_o$) to the page (30 cm × 21 cm)]. All columns must be headed. A ' paste-up ' on white card of computer printout will be acceptable providing the quality of the printout is adequate.

# NOTICE TO AUTHORS—No. 9/1974

## Nomenclature

For many years the Society has actively encouraged the use of standard I.U.P.A.C. nomenclature and symbolism in its publications as an aid to the accurate and unambiguous communication of chemical information between authors and readers. Although the I.U.P.A.C. rules for naming organic compounds have now gained wide acceptance amongst chemists, mainly because they have been in existence for a number of years, those for naming inorganic compounds are of more recent origin and for this reason their acceptance is less general.

In order to encourage authors to use I.U.P.A.C. nomenclature rules when drafting papers, attention is drawn to the following publications in which both the rules themselves and guidance on their use are given.

'Nomenclature of Organic Chemistry, Sections A, B, and C,' Butterworths, London, 2nd Edition, 1971.

'Nomenclature of Inorganic Chemistry,' Butterworths, London, 1971.

'Manual of Symbols and Terminology for Physicochemical Quantities and Units,' Butterworths, London, 1970.

In addition to the above publications, provisional rules for the naming of organometallic compounds, amino-acids, carbohydrates, carotenoids, and steroids, and rules of stereochemistry are available from the:

I.U.P.A.C. Secretariat,
Bank Court Chambers,
2—3 Pound Way,
Cowley Centre,
OXFORD OX4 3YF.

It is recommended that where there are no I.U.P.A.C. rules for the naming of particular compounds or authors find difficulty in applying the existing rules, they should seek the advice of the Society's editorial staff.

# NOTICE TO AUTHORS—No. 10/1976

## Authentication of New Compounds

(1) It is the responsibility of authors to provide fully convincing evidence for the homogeneity and identity of all compounds they claim as new. Evidence of both purity and identity is required to establish that the properties and constants reported are those of the compound with the new structure claimed.

(2) In the context of this Notice a compound is considered as new (*a*) if it has not been prepared before, (*b*) if it has been prepared before but not adequately purified, (*c*) if it has been purified but not adequately characterised, (*d*) if, earlier, it has been assigned an erroneous constitution, or (*e*) if it is a natural product synthesised for the first time. In preliminary communications compounds are often recorded with limited characterising data; in spite of (*c*) above later preparations of such compounds are not considered as new if the properties previously reported are confirmed; the same applies to patents.*

(3) Referees are asked to assess, as a whole, the evidence in support of the homogeneity and structure of all new compounds. No hard and fast rules can be laid down to cover all types of compounds, but the Society's policy remains unchanged in that evidence for the unequivocal identification of new compounds should normally include good elemental analytical data; an accurate mass measurement of a molecular ion does not provide evidence of purity of a compound and must be accompanied by independent evidence of homogeneity. Low-resolution mass spectroscopy must be treated with even more reserve in the absence of firm evidence to distinguish between alternative molecular formulae. Where elemental analytical data are not available, appropriate evidence which is convincing to an expert in the field will be acceptable, but authors should include, for the referees, a brief explanation of the special nature of their problem.

(4) Spectroscopic information necessary to the assignment of structure should normally be given. Just how complete this information should be must depend upon the circumstances; the structure of a compound obtained from an unusual reaction or isolated from a natural source needs much stronger supporting evidence than one derived by a standard reaction from a precursor of undisputed structure. Authors are reminded that full spectroscopic assignments may always be treated as a Supplementary Publication where their importance does not justify their inclusion in the published paper.

(5) Finally, referees are reminded of the need to be exacting in their standards but at the same time flexible in their admission of evidence. It remains the Society's policy to accept work only of high quality and to permit no lowering of present standards.

* New compounds should be indicated by underlining the name (for italics) at its first mention (excluding headings) in the Experimental section only, and by giving analytical results in the form: (Found: C, 63.1; H, 5.4. $C_{13}H_{13}NO_4$ requires C, 63.2; H, 5.3%). If analytical results for compounds which have been adequately described in the literature are to be included, they should be given in the form: (Found: 62.95; H, 5.4. Calc. for $C_{13}H_{13}NO_4$: C, 63.2; H, 5.3%). Analyses are normally quoted to the nearest 0.05%.

# NOTICE TO AUTHORS—No. 11/1976

## Publication of *X*-Ray Crystallographic Work in the *Journal*

### Preamble

At a meeting of the Primary Journals Committee held in October 1975 a sub-committee was set up to consider policy with regard to publication in the *Journal* of both preliminary communications and substantive papers concerned with *X*-ray crystallographic work. This step was taken in the light of correspondence received by the Society which indicated concern by many referees on the problems created by the large number of routine *X*-ray crystallographic studies submitted to the Society as a result of the increasing ease of carrying out such work.

Since the sub-committee's terms of reference were wide it was able to consider both this problem and others relating to publication of *X*-ray crystallographic work in all sections of the *Journal*. Its recommendations which are outlined below fall into two groups: those concerned with preliminary communications and those with full papers. These recommendations have been endorsed by the Primary Journals Committee and now represent the Society's policy with regard to crystallographic work submitted for publication in its primary journals.

### Preliminary Communications

(1) Evidence was presented to the sub-committee that a major problem associated with the publication of preliminary reports of crystallographic work in *J.C.S. Chem. Comm.* arose as a result of the non-availability to interested readers of the atomic co-ordinates associated with this work. Although in the normal course of events such data would be expected to appear in the follow-up paper, many cases were cited where the period between publication of the preliminary report and the substantive paper was many years or the full papers never appeared in print. The evidence presented suggested that there was considerable disquiet among crystallographers at this state of affairs. In an attempt to improve this situation and after consultation with the Cambridge Crystallographic Data Centre (C.C.D.C.) the Society has resolved to press authors of preliminary reports of *X*-ray crystallographic work to submit together with their communication certain material for deposition with the Centre.* This material will be checked at the Centre for internal consistency and, afterwards, will be available on request to interested readers. The procedure to be adopted will be as follows:

(i) In addition to the communication and the customary covering letter of justification the authors will be expected to provide a complete list of refined co-ordinates (in the form of computer print-out and NOT a retyped version) and a table of bond distances unless these are given in full in the manuscript. If the complete 'crystal data' (*i.e.* cell dimensions and standard deviations, space group, number *Z* of formulae units per cell) are not listed in the manuscript these must also be submitted.

It should be emphasised that the co-ordinates submitted for deposition, whilst not necessarily being 'fully' refined, should correspond to the stage of refinement described in the preliminary communication and should be the set for which the *R* factor is quoted. It follows that all bond distances given in the preliminary communication should correspond, apart from any rounding-off errors, with bond distances which can be calculated from the deposited co-ordinates.

(ii) The communication will be assessed in the customary fashion, the material for deposition also being made available to the referees concerned. If the communication is accepted the Society will forward the material for deposition to the C.C.D.C. A statement will be made in the communication that particular material is available from the Centre on request.

(iii) The C.C.D.C. will acknowledge receipt of the material. When a communication is published the deposited material will be evaluated and included in their files as part of their normal abstracting cycle. The evaluation consists of recalculation of the bond lengths from the author's co-ordinates and comparison of these with the author's values. All data on the Centre's files have to pass this internal consistency test. It will not, however, be possible for the evaluation to be made before the appearance of the preliminary communication in print.

(iv) Finally, where an author plans not to follow-up his preliminary communication with a full paper he will be required to submit, in addition to the material outlined above, a copy of the structure factor table for the work presented for deposition with the British Library, Lending Division. In this way it too will be available to interested readers.

(2) In order to aid the readability of communications it is recommended that each should contain a line drawing of the compound under discussion where appropriate.

### Papers in Dalton and Perkin Transactions

The sub-committee considered evidence which indicated that *X*-ray crystallographic papers submitted to the *Journal* were assessed in a less rigorous fashion than those reporting other areas of work. Although the sub-committee felt that this claim was largely unsubstantiated it was agreed that improvement of both assessment procedure and presentation of work was possible. The following recommendations have, therefore, been adopted.

(1) Crystallographic papers will be assessed for their chemical as well as their crystallographic interest.

(2) Unless both specifically requested by the author and recommended by the referees for publication, vibrational parameters will be routinely deposited with the structure factors as a Supplementary Publication. Where vibrational parameters are to be published they should be in the form of $U_{ij}$ with units of Å$^2$.

Referees are reminded that they may, at their discretion, recommend other material for deposition where in their view its inclusion in the parent paper is not justified by its interest.

(3) Each paper should contain a line drawing of the compound under discussion where appropriate in addition to the usual crystallographic figures.

* Applies only to compounds containing organic carbon atoms.

## NOTICE TO AUTHORS—No. 12/1977

### Publication of Theoretical and Computational Papers

The Primary Journals Committee has been considering future policy towards the publication of papers with a heavily computational content, particularly where these involve standard methods, such as semi-empirical or *ab initio* calculations of molecular electronic properties using readily available computer programmes. Many such papers report what would be considered 'routine work' in other areas of chemistry, and have often included extensive detail.

A specialist sub-committee formulated a set of proposals which were circulated to a large representative sample of theoretical chemists and met with general acceptance. These, with the comments on them, form the basis of this notice.

The Primary Journals Committee recognises that computational work can play a valuable role in chemistry, and will probably continue to do so on an increasing scale. It accepts the time-honoured principle that the first criterion for publication of a paper by the Society should be the worthiness of the chemical problem considered, rather than the particular techniques employed by the author. For example, the use of a new computing algorithm, or the modification of a programme, would not usually, on its own, provide sufficient justification for publication.

The Primary Journals Committee recommends to authors the following guidelines for the preparation of computational papers, so that the material can be presented concisely and effectively.

(i) Papers should be submitted to the appropriate journal: a paper containing innovations in theory to Faraday Transactions II, one in which the computations are incidental to the chemistry to Perkin, Dalton, or Faraday I Transactions. Papers concerned mainly with computational details are unlikely to be accepted.

(ii) The purpose of the paper and the precise objectives of the calculations performed should be clearly stated: the results obtained should be reported only in so far as they relate to those objectives.

(iii) Many papers use a routine procedure based on a well documented method, be it semi-empirical or *ab initio*. It is then sufficient to name the particular variant, referring to key papers in which the method was developed, to cite the computer programme used, and to indicate *briefly* any modification made by the author. A review of theoretical background would be out of place, but an author should say why he considers the method adequate for his purposes.

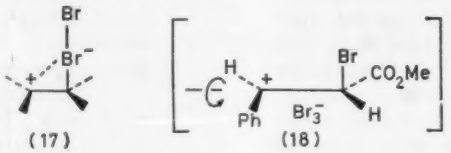
(iv) Extensive tabulation of numerical results, such as the magnitudes of atomic orbital coefficients, electron populations, contour maps of molecular orbitals and electron densities, and peripheral material of a similar nature, is normally unnecessary. Lengthy line-by-line discussion of such material is, as a general rule, quite unacceptable. Where an author considers that there is a special need to make such material available to other workers, as with highly accurate computations, for example, then this may be deposited with the British Library as a Supplementary Publication. Such material should be submitted with the main paper, clearly distinguished from it, and referred to in the main text.

Guidelines can never provide sufficient criteria for acceptance or rejection of a paper. Critical assessment of the theoretical methods used in a computation, and of their suitability for the purpose in hand, will continue to be entrusted to specialist referees who must also decide whether the results are new and advance science.

# ERRATA

## Perkin II Transactions

1976, page 146, left-hand column: *delete* block of formulae and *insert* the following:




page 146, right-hand column, paragraph 3, opening sentence: *delete* ' Yates and McDonald [40] . . . reaction pathway ' and *insert* ' Yates and McDonald [40] suggest that cyclic transition states are involved in additions to stilbene even if non-bridged intermediates are formed further along the reaction pathway.'

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1977, page 430, left-hand column: in Table 1 *delete* second and fourth entries ' 8.81 and 21.4; and 1.48 and 3.60 ' and *insert* ' 1.48 and 3.60; and 8.81 and 21.4 ' respectively; line 21 *delete* ' (1a) and (3a) ' and *insert* ' (1b) and (3b) '; line 22 *delete* ' (2a) ' and *insert* ' (2b) '; line 24 *delete* '( 1b) and (3b) ' and *insert* ' (1a) and (3a) '; line 25 *delete* ' (2b) ' and *insert* ' (2a) '.

page 430, right-hand column, lines 14 and 15: *delete* ' This could . . . reduce the rate ' and *insert* ' Relief of strain in the decomposition of the chromate ester of this compound could increase the rate.'

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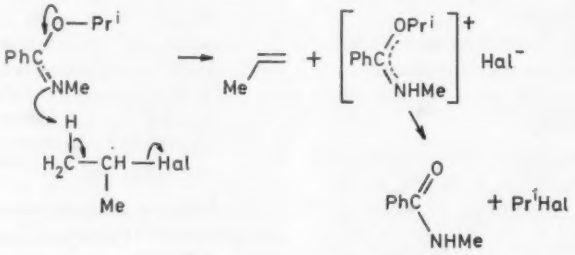
1978, page 102, Table 5: the signals for (14a; X = H) at C-9a and C-9b of 111.6 is due to an impurity; the signals for (14b; X = H) at C-1 and C-2 should be *interchanged* as should those for C-8 and C-9.

page 103, Table 7: fourth column *delete* ' 100 [b] ' and *insert* ' 100 [b,32] '; footnote *d*, *delete* ' ref. 32 ' and *insert* ' ref. 23 '.

page 196: *delete* Scheme 3 and *insert* the following:

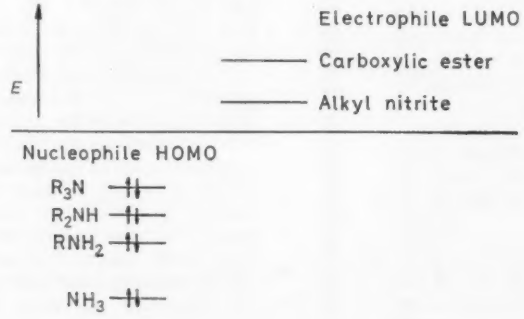



page 369; Figure 1: The atom numbering in Figure 1 is correct, but the atom labelling is incorrect. The correct sequence of atoms should be: O(1), C(2), C(3), C(4), C(5), C(6), C(7), N(8), C(9), C(10), C(11), C(12), C(13), C(14), C(15), O(16), and C(17).

page 454, left-hand column: at foot of page *insert* reference 5 as follows: ' M. Suama, T. Sugita, and K. Ichikawa, *Bull. Chem. Soc. Japan.*, 1971, **44**, 1999.'

page 790, right-hand column: *delete* equation (8) and '*insert* $[C_A\text{-}(x,t + \Delta t) - C_A\text{-}(x,t)]/\Delta t$.

page 1128, left-hand column: *delete* Figure 4 and *insert* the following:



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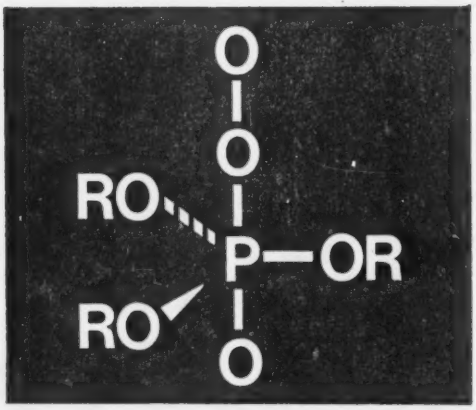


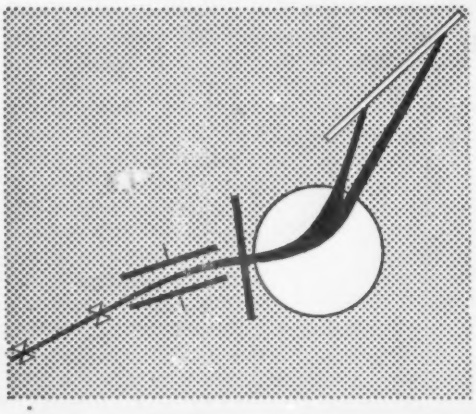

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